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THEORY OF THE PHOTOELECTRIC EFFECT

I. FORMAL ASPECTS

M. E. Rose
L. C. Biedenharn

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THEORY OF THE PHOTOELECTRIC EFFECT. I. FORMAL ASPECTS

M. E. Rose and L. C. Biedenharn*

I. INTRODUCTION

The need for an essentially exact calculation of the photoelectric cross section has been felt for some time. The quantities of interest are:

(1) The total cross section for an adequate number of values of Z and for energies in the region where relativistic effects cannot be neglected.

(2) The angular distribution with unpolarized radiation as a function of Z and energy.

(3) The angular distribution with linearly polarized radiation, or more particularly, the asymmetry ratio for a given angle of emergence of the photoelectron and as a function of Z and energy. The asymmetry ratio is defined as the ratio of differential cross sections for ejection in the plane of polarization and orthogonal to that plane.[1]

At present there are a number of approximate calculations available.[2]

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*Summer visitor, Yale University. Now at Rice Institute, Houston, Texas.

[1]W. H. McMaster and F. L. Hereford, Phys. Rev. 95, 723 (1954). This paper presents the only experimental material on the polarization asymmetry of which we are aware.

[2]Born Approximation, P. Sauter, Ann d. Phys. 11, 454 (1931); A. Sommerfeld, Atombau und Spektrallinien(F. Vieweg und Sohn, Braunschweig, 1939) Vol. 2, p. 482. High energy limit, for the total cross section, H. Hall, Rev. Mod. Phys. 8, 358 (1936).

The only relativistic calculation wherein the Coulomb field is taken into account was made by Hulme et al.[3] Only the total cross section was considered and results are given for the K-shell alone. No screening effects were allowed for. Whether or not this is a good approximation, even for the K-shell, remains to be seen. Experience indicates that in a very similar situation, the internal conversion process, screening may make a difference of 10 percent or less. For the photoelectric effect one might expect somewhat larger effects because larger values of r are effective. This difference arises from the circumstance that in the internal conversion outgoing waves are involved and these are singular at the origin while in the photoelectric effect only standing waves enter and the origin contributes very little.

It is clear that the calculation of the photoelectric cross-section is a formidable task even if one confines the work to the K-shell. However, it seems that the order of magnitude of the task involved in calculating the angular distribution is not much greater than that involved in the total cross section. It is quite certain that it is no more difficult to include the effect of polarization than it is to ignore it. In any event it is our purpose in this report to exhibit the form of the cross-section in order to provide a basis for assessing and organizing a calculational program. It

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[3] H. R. Hulme et al, Proc. Roy. Soc. (London) 149, 131 (1935).

is emphasized that this report does not contain numerical results. It is hoped that it will be possible to present such results at a later time.

II. GENERAL FORM OF THE CROSS-SECTION

(a) The wave functions and radiation field.

For ejection from the subshell i we designate the cross-section by σ_i. The cross-section for all subshells will be

$$\sigma = \sum_i \sigma_i \tag{1}$$

summed over all pertinent subshells. The cross-section σ_i is found from

$$\sigma_i = \mathcal{S}\ r^2\ \frac{j_{out}}{j_{in}} \tag{2}$$

where j_{out} is the current density for a Dirac electron with a direction of propagation defined asymptotically by polar angles ϑ, φ ; j_{in} is the photon flux of the incident radiation and $\mathcal{S}$ implies an averaging (and/or summation) over unobserved parameters. For example, $\mathcal{S}$ will involve

$$\frac{n_i}{2j_i+1} \sum_m \tag{3}$$

where n_i is the number of electrons in subshell i, j_i the angular momentum for this subshell and m is the corresponding magnetic quantum number.

The outgoing current is

$$j_{out} = -(\Psi, \alpha_r \Psi) \tag{4}$$

where round brackets imply only a spinor sum - no integration over angles. The construction of an electron wave function for a central field problem where the direction of motion is asymptotically defined has been carried out elsewhere.[4] For large r this is

$$\Psi \to i\sqrt{\pi}\,\frac{e^{ipr}}{r}\sum_{\chi_\mu} e^{i\Delta_\kappa}\, S_\kappa \langle \Phi_\kappa^\mu | \mathcal{H} | \Phi_i \rangle \times \begin{pmatrix} -i\, S_\kappa \sqrt{\frac{W-1}{p}}\, \chi_{-\kappa}^\mu \; e^{-\frac{1}{2}\pi i(1+\ell_{-\kappa})} \\ \sqrt{\frac{W+1}{p}}\, \chi_\kappa^\mu \; e^{-\frac{1}{2}\pi i(1+\ell_\kappa)} \end{pmatrix} \tag{5}$$

Here W and p are the energy (including rest energy) and momentum at infinity. The units used throughout are $m = c = \hbar = 1$. In (5) as elsewhere the angular brackets imply coordinate integration as well as spinor summation. Φ_i is the initial state wave function and for the final state one writes

$$\Phi_\kappa^\mu = \begin{pmatrix} -i\, f_\kappa \chi_{-\kappa}^\mu \\ g_\kappa \chi_\kappa^\mu \end{pmatrix} \tag{6}$$

where f_κ, g_κ are radial functions normalized per unit energy interval.[5] These fulfill the differential equations (consistent with the representation $\vec{\alpha} = \rho_1 \vec{\sigma}$ and the sign in (4))

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[4] M. E. Rose, L. C. Biedenharn and G. B. Arfken, Phys. Rev. 85, 5 (1952); referred to as RBA.

[5] For the Coulomb field these are given explicitly by M. E. Rose, Phys. Rev. 51, 484 (1937).

$$\frac{df}{dr} = \frac{\varkappa + 1}{r} f - (W - 1 - V)g \tag{7a}$$

$$\frac{dg}{dr} = (W + 1 - V)f - \frac{\varkappa - 1}{r} g \tag{7b}$$

where V is an arbitrary central field. Also $\varkappa$ is a non-vanishing integer, with the total angular momentum of the electron given by

$$j = |\varkappa| - \tfrac{1}{2} \tag{8}$$

and

$$\ell_\varkappa = \varkappa \quad \text{for} \quad \varkappa > 0 \tag{9a}$$

$$= -\varkappa - 1 \quad \text{for} \quad \varkappa < 0 \tag{9b}$$

Thus

$$\ell_{-\varkappa} = \ell_\varkappa - S_\varkappa \tag{10}$$

where $S_\varkappa$ is the sign of $\varkappa$, (see Table I for particular examples). The wave function Φ_i is defined as in (6) but with $\varkappa$, μ replaced by $\varkappa_i$, m. In (6) the $\chi_\varkappa^\mu$ are Pauli spin-angular spinors defined by

$$\chi_\varkappa^\mu = \sum_\tau C(\ell_\varkappa \tfrac{1}{2} j; \mu - \tau, \tau)\, Y_{\ell_\varkappa}^{\mu-\tau} \chi_{\frac{1}{2}}^{\tau} \tag{11}$$

$$\chi_{\frac{1}{2}}^{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\frac{1}{2}}^{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The C-coefficient is a vector addition coefficient and μ is the magnetic quantum number. Finally, in (5) $\mathcal{H}$ is the perturbation due to the radiation, i.e.,

$$\mathcal{H} = e\, \vec{\alpha} \cdot \vec{A} \tag{12}$$

with $\vec{A}$ the vector potential of the radiation; Δ_κ is the phase shift due to V. Thus,[6]

$$f_\kappa(\infty) = -\sqrt{\frac{p}{\pi}(W-1)} \lim_{r\to\infty} j_{\ell_{-\kappa}}(pr + \Delta_\kappa) \tag{13a}$$

$$g_\kappa(\infty) = -\sqrt{\frac{p}{\pi}(W+1)}\, S_\kappa \lim_{r\to\infty} j_{\ell_\kappa}(pr + \Delta_\kappa) \tag{13b}$$

with $j_\lambda(pr)$ the spherical bessel function. For the Coulomb field

$$\Delta_\kappa = \delta_\kappa(Z) - \delta_\kappa(0) \tag{14}$$

where

$$\delta_\kappa(Z) = \eta_\kappa - \frac{\pi\gamma_\kappa}{2} - \arg\Gamma(\gamma_\kappa + i\alpha ZW/p) \tag{14a}$$

and

$$2\eta_\kappa = \arg\frac{-\kappa + i\alpha Z/p}{\gamma_\kappa + i\alpha ZW/p} \tag{14b}$$

$$\gamma_\kappa = \sqrt{\kappa^2 - \alpha^2 Z^2} \quad ; \qquad \alpha \cong 1/137. \tag{14c}$$

From (4) and (5) we find

$$\begin{aligned} r^2 j_{out} = \pi i \sum_{\kappa\kappa'}\sum_{\mu\mu'} & e^{i(\Delta_\kappa - \Delta_{\kappa'})} S_\kappa S_{\kappa'} \langle \kappa'\mu' | \mathcal{H} | \Phi_i \rangle^* \\ & \times \langle \kappa\mu | \mathcal{H} | \Phi_i \rangle (\chi^{\mu'}_{\kappa'}, \chi^{\mu}_{\kappa}) \Big[S_\kappa e^{\frac{1}{2}\pi i(\ell_{\kappa'} - \ell_{-\kappa})} (\chi^{\mu'}_{\kappa'}, \sigma_n \chi^{\mu}_{-\kappa}) \\ & - S_{\kappa'} e^{\frac{1}{2}\pi i(\ell_{-\kappa'} - \ell_\kappa)} (\chi^{\mu'}_{-\kappa'}, \sigma_n \chi^{\mu}_{\kappa}) \Big] \end{aligned} \tag{15}$$

---

[6] Strictly speaking, $\delta_\kappa(Z)$ and hence Δ_κ should contain the logarithmic term $\frac{\alpha ZW}{p}\log 2pr$. However, only phase differences $\Delta_\kappa - \Delta_{\kappa'}$ will be relevant and this term drops out as usual.

Using

$$\sigma_r \chi^{\mu}_{\varkappa} = - \chi^{\mu}_{-\varkappa} \tag{16}$$

so that

$$(\chi^{\mu'}_{-\varkappa'}, \sigma_r \chi^{\mu}_{\varkappa}) = - (\chi^{\mu'}_{-\varkappa'}, \chi^{\mu}_{-\varkappa}) = - (\chi^{\mu'}_{\varkappa'}, \chi^{\mu}_{\varkappa}) = (\chi^{\mu'}_{\varkappa'}, \sigma_r \chi^{\mu}_{-\varkappa}) \tag{16a}$$

and

$$S_{\kappa'} e^{\frac{1}{2}\pi i(\ell_{-\kappa'} - \ell_{\kappa})} = - S_{\kappa} \; e^{\frac{1}{2}\pi i(\ell_{\kappa'} - \ell_{-\kappa})} \tag{16b}$$

we find from (10) that[7]

$$r^2 j_{out} = 2\pi \sum_{\varkappa\varkappa'} \sum_{\mu\mu'} e^{i(\Delta_{\varkappa} - \Delta_{\varkappa'})} S_{\varkappa} S_{\varkappa'} \; e^{\frac{1}{2}\pi i(\ell_{\kappa'} - \ell_{\kappa})}$$
$$\times \langle \varkappa'\mu' | \mathcal{H} | \Phi_i \rangle^* \langle \varkappa\mu | \mathcal{H} | \Phi_i \rangle (\chi^{\mu'}_{\varkappa'}, \chi^{\mu}_{\varkappa}) \tag{17}$$

As a check we consider the total cross-section $\bar{\sigma}_i$. Integrating over ϑ, φ we have

$$\langle \chi^{\mu'}_{\varkappa'}, \chi^{\mu}_{\varkappa} \rangle = \delta_{\varkappa'\varkappa} \, \delta_{\mu'\mu} \tag{18}$$

so that

$$\bar{\sigma}_i = \frac{2\pi}{j_{in}} S \sum_{\kappa\mu} |\langle \varkappa\mu | \mathcal{H} | \Phi_i \rangle|^2 \tag{19}$$

as expected. This also verifies the statement made above concerning the normalization of the final state radial wave functions.

---

[7]The difference between (17) and Eq. (25) of RBA is a factor - 2π which was irrelevant for the purposes of that paper.

The vector potential $\vec{A}$ of Eq. (12) may be written in the form

$$\vec{A} = \frac{1}{\sqrt{2}} \sum_P e^{-iP\xi} \vec{A}_P = \vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}} \tag{20}$$

where $P = \pm 1$ and $\vec{A}_P$ corresponds to a pure circularly polarized wave. That is, with $\vec{k}$ the propagation vector along the z-axis,

$$\vec{A}_P = \frac{\vec{u}_x + iP\vec{u}_y}{\sqrt{2}}\, e^{i\vec{k}\cdot\vec{r}} \tag{21}$$

where $\vec{u}_x$ and $\vec{u}_y$ are unit vectors along the x and y-axes respectively and the unit polarization vector is

$$\vec{\epsilon} = \vec{u}_x \cos\xi + \vec{u}_y \sin\xi \tag{22}$$

The angle ξ is defined with respect to an arbitrary plane through the vector $\vec{k}$. One then finds immediately that

$$j_{in} = \frac{k}{2\pi} \tag{23}$$

For our purpose it is necessary to expand the plane wave into multipole solutions. In the solenoidal gauge these are[8]

$$\vec{A}^M_L(m) = -\sqrt{\frac{2}{\pi}}\; j_L\, \vec{T}^M_{LL} \tag{24}$$

---

[8] See M. E. Rose, Multipole Fields, John Wiley and Sons, New York, 1954. This reference is designated as R.

for a magnetic 2^L pole and

$$\vec{A}^M_L(e) = \sqrt{\frac{2}{\pi}} \left[- \sqrt{\frac{L}{2L+1}}\, j_{L+1}\, \vec{T}^M_{LL+1} + \sqrt{\frac{L+1}{2L+1}}\, j_{L-1} \vec{T}^M_{LL-1} \right] \tag{25}$$

and $\vec{T}^M_{L\lambda}$ are the irreducible tensors defined by

$$\vec{T}^M_{L\lambda} = \sum_{m'} C(1\lambda L; -m', m'+M)\, Y^{M+m'}_{\lambda}\, \vec{u}_{-m'} \tag{26}$$

$$\vec{u}_{\pm 1} = \mp \frac{1}{\sqrt{2}} (\vec{u}_x \pm i\vec{u}_y); \quad \vec{u}_o = \vec{u}_z \tag{26a}$$

No loss of generality is incurred by choosing the quantization axis along $\vec{k}$. Then M = P and (see R, Chapter VI)

$$\vec{A}_P = \pi \sum_{L=1}^{\infty} i^L \sqrt{2L+1} \left[\vec{A}^P_L(m) + i\, P\, \vec{A}^P_L(e) \right] \tag{27}$$

(b) <u>The matrix elements</u>.

We have now defined all the quantities entering in the cross section and at this point one must calculate the matrix elements entering in (17). For this purpose we define reduced matrix elements Q by

$$\langle \chi^{\mu}_{\kappa}, T^P_{L\lambda}\, \chi^{m}_{\bar{\kappa}} \rangle \equiv C(L\bar{j}j; Pm)\ \delta_{\mu, P+m}\ Q(\kappa\bar{\kappa}\ ; \lambda L) \tag{28}$$

These reduced matrix elements are now obtained by calculating the left hand side of (28) which is

$$\sum_M C(1\lambda L; -M\ P+M)\ \langle \chi^{\mu}_{\kappa} | Y^{P+M}_{\lambda}\, \sigma_{-M} | \chi^{m}_{\bar{\kappa}} \rangle \tag{28a}$$

The matrix elements needed are then

$$\langle \varkappa \mu | \mathcal{H} | \Phi_i \rangle = \sqrt{\pi\alpha} \sum_{PL} i^{L+1} \sqrt{2L+1}\, e^{-iP\xi}\, C(Lj_i j;Pm)\, \delta_{\mu,P+m}$$

$$\times \Big\{ - R_L(\varkappa\varkappa_i)\, Q(-\varkappa\, \varkappa_i;LL) + \bar{R}_L(\varkappa\varkappa_i)\, Q(\varkappa, -\varkappa_i;LL)$$

$$+ iP \Big[- \sqrt{\frac{L}{2L+1}} \Big(R_{L+1}(\varkappa\varkappa_i)\, Q(-\varkappa, \varkappa_i;L+1\ L) - \bar{R}_{L+1}(\varkappa\varkappa_i)\, Q(\varkappa, -\varkappa_i;L+1\ L) \Big)$$

$$+ \sqrt{\frac{L+1}{2L+1}} \Big(R_{L-1}(\varkappa\varkappa_i)\, Q(-\varkappa, \varkappa_i;L-1\ L) - \bar{R}_{L-1}(\varkappa\varkappa_i)\, Q(\varkappa, -\varkappa_i;L-1\ L) \Big) \Big] \Big\} \quad (29)$$

with[9]

$$R_\lambda(\varkappa\varkappa_i) = \int_0^\infty r^2 f_\varkappa\, j_\lambda\, g_{\varkappa_i}\, dr$$

$$\bar{R}_\lambda(\varkappa\varkappa_i) = \int_0^\infty r^2 g_\varkappa\, j_\lambda\, f_{\varkappa_i}\, dr$$

To calculate the (angular bracket) matrix element in (28a) we write it in the form, see Eq. (11),

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[9] If comparison is made with the closely associated problem of internal conversion, M. E. Rose, G. H. Goertzel, B. I. Spinrad, J. Harr and P. Strong, Phys. Rev. 83, 79 (1951), it is seen that the latter involves radial integrals with $f_\varkappa f_{\varkappa_i}$ and $g_\varkappa g_{\varkappa_i}$. The distinction lies in the gauge. While any gauge is suitable the most convenient gauge in the internal conversion is the non-solenoidal one with the $\vec{T}_{L,L+1}$ terms absent. This is connected with the important distinction that in internal conversion outgoing and not standing waves are necessary, see R. Chap. V.

$$\left\langle \chi^{\mu}_{\varkappa},\ Y^{P+M}_{\lambda}\,\sigma_{-M}\,\chi^{m}_{\bar{\varkappa}} \right\rangle = \sum_{\tau\bar{\tau}} C(\ell\,\tfrac{1}{2}j;\mu-\tau\ \ \tau)\ C(\bar{\ell}\,\tfrac{1}{2}\bar{j};m-\bar{\tau},\bar{\tau})$$

$$\times\ (\chi^{\tau}_{\frac{1}{2}},\ \sigma_{-M}\,\chi^{\bar{\tau}}_{\frac{1}{2}})\left\langle Y^{\mu-\tau}_{\ell},\ Y^{P+M}_{\lambda}\,Y^{m-\bar{\tau}}_{\bar{\ell}} \right\rangle$$

Here $\ell \equiv \ell_{\varkappa}$, $\bar{\ell} \equiv \ell_{\bar{\varkappa}}$; $j \equiv j_{\varkappa}$ and $\bar{j} \equiv j_{\bar{\varkappa}}$. Using the result (R, Eq. (2.33))

$$\left\langle Y^{\mu-\tau}_{\ell},\ Y^{P+M}_{\lambda}\,Y^{m-\bar{\tau}}_{\bar{\ell}} \right\rangle$$

$$= \sqrt{\frac{(2\lambda+1)(2\bar{\ell}+1)}{4\pi(2\ell+1)}}\ C(\lambda\,\bar{\ell}\,\ell\,;00)\ C(\lambda\,\bar{\ell}\,\ell;P+M,m-\bar{\tau})\ \delta_{\mu-\tau,P+M+m-\bar{\tau}} \qquad (28b)$$

and

$$(\chi^{\tau}_{\frac{1}{2}},\ \sigma_{-M}\,\chi^{\bar{\tau}}_{\frac{1}{2}}) = (-)^{M}\ \sqrt{3}\ C(\tfrac{1}{2}\ 1\tfrac{1}{2};\bar{\tau}-M,M)\ \delta_{\tau,\bar{\tau}-M}$$

We find after two straightforward Racah recouplings[10]

$$\left\langle \chi^{\mu}_{\varkappa},\ Y^{P+M}_{\lambda}\,\sigma_{-M}\,\chi^{m}_{\bar{\varkappa}} \right\rangle = \sqrt{\frac{3}{2\pi}\,(2\lambda+1)(2\bar{\ell}+1)(2\bar{j}+1)}\ (-)^{\bar{\ell}+\bar{j}-\frac{1}{2}}$$

$$\times\ C(\lambda\,\bar{\ell}\,\ell\,;00)\ \sum_{s}\sqrt{2s+1}\ W(\lambda\bar{\ell}\,j\tfrac{1}{2};\ell\,s)\ W(\bar{j}\tfrac{1}{2}s\tfrac{1}{2};\bar{\ell}\,1)$$

$$\times\ C(\lambda s j;P+M,m-M)\ C(\bar{j}1s;m,-M)$$

From (28a) another Racah recoupling permits the M summation to be carried out yielding

---

[10] See RBA, Appendix B, Eq. (B.3).

$$Q(\varkappa\bar{\varkappa};\lambda L) = \sqrt{\frac{3}{2\pi}(2L+1)(2\lambda+1)(2\bar{\ell}+1)(2\bar{j}+1)}\ (-)^{\ell+j-\bar{\ell}-\bar{j}}\ C(\lambda\bar{\ell}\ell;00)$$

$$\times\ X(Lj\bar{j};\lambda\ell\bar{\ell};1\tfrac{1}{2}\tfrac{1}{2}) \tag{30}$$

wherein the X-coefficient defined by[11]

$$X(abc;def;ghi) = (-)^{\sigma}\sum_{s}(2s+1)\ W(bdcg;sa)\ W(dbfh;se)\ W(gchf;si)$$

$$\sigma = a + b + c + d + e + f + g + h + i$$

has been introduced. Actually this X-coefficient which, incidentally, defines the recoupling from j-j to L-S coupling schemes for two particles of intrinsic spin $\frac{1}{2}$, constitutes a degenerate case. That is, it can be rather simply expressed in terms of a single Racah coefficient. This is demonstrated in the appendix. The results given there show that

$$X(Lj\bar{j};L\ell\bar{\ell};1\tfrac{1}{2}\tfrac{1}{2}) = \frac{(-)^{j+\ell+\frac{1}{2}}(\varkappa-\bar{\varkappa})}{\sqrt{6L(L+1)(2L+1)}}\ W(\bar{\ell}\bar{j}\ell j;\tfrac{1}{2}L) \tag{31a}$$

$$C(L+1,\bar{\ell}\ell;00)\ X(Lj\bar{j};L+1\ \ell\bar{\ell};1\tfrac{1}{2}\tfrac{1}{2}) = \frac{(-)^{j+\ell+\frac{1}{2}}(\varkappa+\bar{\varkappa}+L+1)}{\sqrt{6(L+1)(2L+1)(2L+3)}}\ C(L\ \bar{\ell}\ \ell_{-\kappa};00)$$

$$\times\ W(\bar{\ell}\bar{j}\ \ell_{-\kappa}\ j;\tfrac{1}{2}L) \tag{31b}$$

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[11] U. Fano and G. Racah, unpublished. See also U. Fano, Nat. Bur. of Stand. Report No. 1214, p. 48.

$$C(L\text{-}1\ \bar{\ell}\ \ell;00)\ W(Lj\bar{j};L\text{-}1\ \ell\bar{\ell};1\tfrac{11}{22}) = \frac{(-)^{j+\ell+\frac{1}{2}}\ (\varkappa+\bar{\varkappa}-L)}{\sqrt{6L(2L+1)(2L-1)}}\ C(L\ \bar{\ell}\ \ell_{-\varkappa};00)$$

$$\times\ W(\bar{\ell}\ \bar{j}\ \ell_{-\varkappa}\ j;\tfrac{1}{2}L) \qquad (31c)$$

All these Racah coefficients can be written in elementary form, once the signs of $j - \ell$ and $\bar{j} - \bar{\ell}$ are fixed.[12] The C-coefficients are evaluated from Eq. (5) of BBR.

Note that $C(\alpha\beta\gamma;00) = 0$ unless $\alpha + \beta + \gamma$ is an even integer. This parity rule plays an important role in the following.

(c) <u>The cross-section</u>.

It is now convenient to introduce the magnetic and electric matrix elements according to

$$M_L(\varkappa) \equiv \sqrt{2L+1}\ \left[-\ R_L(\varkappa)\ Q(-\varkappa,\varkappa_i;LL) + \bar{R}_L(\varkappa)\ Q(\varkappa,-\varkappa_i;LL)\right] \qquad (32)$$

and

$$E_L(\varkappa) \equiv -\ \sqrt{L}\ \left[R_{L+1}(\varkappa)\ Q(-\varkappa,\varkappa_i;L+1\ L) - \bar{R}_{L+1}(\varkappa)\ Q(\varkappa,-\varkappa_i;L+1\ L)\right]$$

$$+\ \sqrt{L+1}\ \left[R_{L-1}(\varkappa)\ Q(-\varkappa,\varkappa_i;L\text{-}1\ L) - \bar{R}_{L-1}(\varkappa)\ Q(\varkappa,-\varkappa_i;L\text{-}1\ L)\right] \qquad (33)$$

where, in the interest of simplicity, the $\varkappa_i$ argument has been suppressed

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[12] L. C. Biedenharn, J. M. Blatt and M. E. Rose, Rev. Mod. Phys. 24, 249 (1952). See especially Table I on p. 253. This reference is designated as BBR.

in the radial matrix elements R and $\bar{R}$ as well as in M_L and E_L. Then the cross-section becomes

$$\sigma_i = \frac{4\pi^3\alpha}{k}\,\frac{n_i}{2j_i+1}\sum_{LL'}\sum_{\varkappa\varkappa'} e^{i\Delta_{\varkappa\varkappa'}} S_\varkappa S_{\varkappa'} e^{\frac{1}{2}\pi i(\ell_{\varkappa'}-\ell_\varkappa)}\, e^{i(P'-P)\xi}$$

$$\times\, i^{L-L'}\left[M_L(\varkappa) + iPE_L(\varkappa)\right]\left[M_{L'}(\varkappa') - iP'E_{L'}(\varkappa')\right]\sum_m\sum_{\mu\mu'} C(Lj_ij;Pm\mu)$$

$$C(L'j_ij';P'm\mu')(\chi^{\mu'}_{\varkappa'},\chi^{\mu}_{\varkappa}) \tag{34}$$

We have further abbreviated the notation by defining

$$\Delta_{\varkappa\varkappa'} \equiv \Delta_\varkappa - \Delta_{\varkappa'}$$

and the conservation rules for the magnetic quantum numbers ($P+m = \mu$, $P'+m = \mu'$) are expressed by writing C-coefficients with three magnetic quantum numbers.

To carry out the sums over m, μ and μ' we use

$$(\chi^{\mu}_{\varkappa},\chi^{\mu'}_{\varkappa'}) = (-)^{\mu'+\frac{1}{2}+\nu+j+j'}\sqrt{\frac{(2j+1)(2j'+1)(2\ell+1)(2\ell'+1)}{4\pi(2\nu+1)}}$$

$$\times\sum_\nu C(\ell\ell'\nu;00)\, C(jj'\nu;\mu,-\mu')\, W(\ell\ell'jj';\nu\tfrac{1}{2})\, Y_\nu^{\mu-\mu'}(\vartheta,\varphi)$$

which is obtained from (11), the coupling rule (28b) and a Racah recoupling.[10] We now have the sum

$$\sum_m (-)^{m+\frac{1}{2}}\, C(Lj_ij;Pm)\, C(L'j_ij';P'm)\, C(jj'\nu;P+m,-P'-m)$$

to perform. This again involves a simple Racah recoupling.[10] The result inserted in (34) gives

$$\sigma_i = \frac{4\pi^3\alpha}{k}\,\frac{n_i}{2j_i+1}\,(-)^{j_i+\frac{1}{2}} \sum_{LL'}\sum_{\nu}\sum_{PP'} e^{i\Delta_{\varkappa\varkappa'}} S_\varkappa S_{\varkappa'}$$

$$\times\; e^{\frac{1}{2}\pi i(\ell_{\varkappa'}-\ell_\varkappa)}\, e^{i(P'-P)\xi}\, i^{L-L'} \left[M_L(\varkappa) + iPE_L(\varkappa)\right]\left[M_{L'}(\varkappa') - iP'E_{L'}(\varkappa')\right]$$

$$\times\; (2j+1)(2j'+1)\sqrt{\frac{(2\ell+1)(2\ell'+1)}{4\pi(2\nu+1)}}\; C(\ell\,\ell'\nu;00)\; C(LL'\nu;P-P')\; W(\ell\,\ell' jj';\nu\tfrac{1}{2})\; W(LL'jj';\nu j_i)$$

$$\times\; Y_\nu^{P-P'}(\vartheta\varphi) \qquad (35)$$

The next step is to carry out the P, P' summation. This involves only four terms and is done explicitly. The result is

$$\sigma_i = \frac{\pi^2\alpha\, n_i(-)^{j_i+\frac{1}{2}}}{k(2j_i+1)} \sum_{LL'}\sum_{\varkappa\varkappa'}\sum_{\nu} e^{i\Delta_{\varkappa\varkappa'}} S_\varkappa S_{\varkappa'}\, e^{\frac{1}{2}\pi i(\ell_{\varkappa'}-\ell_\varkappa)}\, i^{L-L'}$$

$$\times\; (2j+1)(2j'+1)\sqrt{(2\ell+1)(2\ell'+1)}\; C(\ell\,\ell'\nu;00)\; W(\ell\,\ell' jj';\nu\tfrac{1}{2})\; W(LL'jj';\nu j_i)$$

$$\times\; \Big\{ C(LL'\nu;1-1)\left[(M_L+iE_L)(M_{L'}-iE_{L'}) + (-)^{L+L'+\nu}\,\text{c.c.}\right] P_\nu$$

$$+\; \sqrt{\frac{(\nu-2)!}{(\nu+2)!}}\; C(LL'\nu;11)\left[(M_L+iE_L)(M_{L'}+iE_{L'})\, e^{2i\beta} + (-)^{L+L'+\nu}\,\text{c.c.}\right] P_\nu^2 \qquad (36)$$

Here

$$\beta = \varphi - \xi$$

and, whereas the first term (multiplying the Legendre polynomial P_ν) in the

curly bracket of (36) represents the polarization-independent part[13], the second term (multiplying the associated Legendre polynomial P_ν^2) is polarization sensitive. Obviously only the difference angle measuring the separation between the electric field and the projection of the electron propagation vector in the plane perpendicular to $\vec{k}$ enters. The asymmetry is the ratio of σ_i for $\beta = 0$ to σ_i for $\beta = \pi/2$.

In (36) we have momentarily dropped the $\varkappa$, $\varkappa'$ arguments from M_L etc. No confusion should result. Also c.c. in each line of the curly bracket is the complex conjugate of the matrix element combination immediately to the left.

We introduce

$$\phi_{\varkappa\varkappa' LL'} = \Delta_{\varkappa\varkappa'} + \frac{\pi}{2}\left(\ell_{\varkappa'} - \ell_{\varkappa} + L - L'\right)$$

---

[13]This part arises from $P = P' = \pm 1$. If we consider circularly polarized radiation the result for the cross-section is obtained from (35) by setting $P = P' = 1$ for left circular polarization (or -1 for right circular polarization) and multiplying by 2 (to remove the factor $1/\sqrt{2}$ in Eq. (20)). It is then fairly evident that the cross-section for circular polarization is exactly the same as for unpolarized radiation: (see discussion leading to Eq. (38) below). This result is to be expected and implies that the detection of circular polarization requires that a direction in space be preferred by polarizing the electron spin in the initial state.

and note that in (36) we may enterchange the summation letters $\varkappa$ and $\varkappa'$ as well as L and L'. Adding the result to (36) and dividing by 2, we find

$$\sigma_i = \frac{\pi^2 \alpha n_i \, (-)^{j_i+\frac{1}{2}}}{k(2j_i+1)} \sum_{LL'} \sum_{\nu} \sum_{\varkappa\varkappa'} (2j+1)(2j'+1) \sqrt{(2\ell+1)(2\ell'+1)}\, S_\varkappa S_{\varkappa'} C(\ell\ell'\nu;00)$$

$$\times\ W(\ell\ell' jj';\nu\tfrac{1}{2})\, W(LL'jj';\nu j_i) \left[\quad\right] \tag{37}$$

where the square bracket is

$$\left[\quad\right] = C(LL'\nu;1\text{-}1)\, P_\nu \Big\{ \cos\phi\ \ (M_L M_{L'} + E_L E_{L'})(1 + (-)^{L+L'+\nu})$$

$$- \sin\phi\ \ (E_L M_{L'} - E_{L'} M_L)(1 - (-)^{L+L'+\nu}) \Big\}$$

$$+ \sqrt{\frac{(\nu-2)!}{(\nu+2)!}}\, C(LL'\nu;11)\, P^2_\nu \Big\{ (M_L M_{L'} - E_L E_{L'}) \left[\cos(\phi + 2\beta) + (-)^{L+L'+\nu} \cos(\phi - 2\beta)\right]$$

$$- (E_L M_{L'} + M_L E_{L'}) \left[\sin(\phi + 2\beta) - (-)^{L+L'+\nu} \sin(\phi - 2\beta)\right] \Big\} \tag{37a}$$

For convenience the subscripts on ϕ are suppressed. The cross-section is now <u>explicitly</u> real.

The second curly bracket of (37a) can be rewritten as

$$= -\sin 2\beta \left[(M_L M_{L'} - E_L E_{L'})(1 - (-)^{L+L'+\nu}) \sin\phi \right.$$

$$\left. + (E_L M_{L'} + M_L E_{L'})(1 + (-)^{L+L'+\nu}) \cos\phi \right]$$

$$+ \cos 2\beta \left[(M_L M_{L'} - E_L E_{L'})(1 + (-)^{L+L'+\nu}) \cos\phi \right.$$

$$\left. - (E_L M_{L'} + M_L E_{L'})(1 - (-)^{L+L'+\nu}) \sin\phi \right] \tag{37b}$$

Remembering the definitions (32) and (33) of M_L and E_L, reference to (30) shows that E_L vanishes unless $\lambda + \ell_{\varkappa_i} + \ell_{-\varkappa} \equiv 0 \pmod 2$ with $\lambda = L \pm 1$ and M_L vanishes unless $\lambda + \ell_{\varkappa_i} + \ell_{-\varkappa} \equiv 0 \pmod 2$ with $\lambda = L$. Hence

$$\lambda + \ell_{\varkappa_i} + \ell_{-\varkappa} \equiv 0 \pmod 2$$

Also

$$\lambda' + \ell_{\varkappa_i} + \ell_{-\varkappa'} \equiv 0 \pmod 2$$

This implies

$$\lambda + \lambda' \equiv \ell_{\varkappa} + \ell_{\varkappa'} \equiv \nu \qquad \pmod 2$$

where the last congruence follows from the parity property of the C-coefficient in (37). We also note that for the self-terms ($M_L M_{L'}$ and $E_L E_{L'}$) $\lambda+\lambda' \equiv L+L'$ (mod 2) while for the interference terms ($M_L E_{L'}$ etc.) $\lambda+\lambda' \equiv L+L'+1$ (mod 2). It then follows that $(-)^{L+L'+\nu} = 1$ for the self-terms and $= -1$ for the interference terms. Hence, all terms in sin 2β in (37b), and therefore in the cross-section, vanish identically. Thus, the cross section is independent of the sign of β. That is, looking along the direction of propagation $\vec{k}$, it does not matter whether the electron is ejected to the left or to the right of the plane of polarization.

With the preceding result we can write $1 \pm (-)^{L+L'+\nu} = 2$ in the surviving terms; i.e., those multiplying cos 2β. Collecting results from (37) and (37b) the cross section is

$$\sigma_i = \frac{2\pi^2 \alpha n_i \, (-)^{j_i+\frac{1}{2}}}{k(2j_i+1)} \sum_{LL'} \sum_{\nu} \sum_{\varkappa\varkappa'} (2j+1)(2j'+1) \sqrt{(2\ell+1)(2\ell'+1)} \; S_\varkappa S_{\varkappa'} C(\ell\ell'\nu;00)$$

$$\times \; W(\ell\ell' jj';\nu\tfrac{1}{2}) \, W(LL'jj';\nu j_i) \Big\{ C(LL'\nu;1\text{-}1) \, P_\nu \Big[\cos\phi \, (M_L M_{L'} + E_L E_{L'})$$

$$- \sin\phi \, (E_L M_{L'} - E_{L'} M_L) \Big]$$

$$+ \sqrt{\frac{(\nu-2)!}{(\nu+2)!}} \; C(LL'\nu;11) \, P^2_\nu \cos 2\beta \Big[\cos\phi \, (M_L M_{L'} - E_L E_{L'})$$

$$- \sin\phi \, (E_L M_{L'} + E_{L'} M_L) \Big] \Big\} \qquad (38)$$

The total cross section is readily obtained by integrating over ϑ, β. The polarization sensitive part obviously makes no contribution and since only $\nu = 0$ contributes, $L = L'$ and $\varkappa = \varkappa'$ are the only surviving terms. Then one finds

$$\bar{\sigma}_i = \int \sigma_i \, d\Omega = \frac{8\pi^3 \alpha n_i}{k(2j_i+1)} \sum_{L\varkappa} \frac{2j+1}{2L+1} \left(M_L^2 + E_L^2\right) \qquad (39)$$

The results given by (38) and (39) represent the final results for the general form of the cross-section. To simplify further, special cases must be considered. This is done in the next section.

III. THE CASE OF $s_{\frac{1}{2}}$ ELECTRONS

The case of greatest interest is the K-shell. Our formal results make no distinction between the K-shell and any other $s_{\frac{1}{2}}$ electron. This distinction appears only when the precise form of the radial integrals is considered. Thus the following would apply to L_I, M_I, N_I etc. electrons.

For $s_{\frac{1}{2}}$ electrons $\varkappa_i = -1$, $\ell_{\varkappa_i} = 0$, $j_i = \frac{1}{2}$. The pertinent $\varkappa$, j, $\ell_\varkappa$ and $\ell_{-\varkappa}$ values are found in Table I. For completeness this table also gives the corresponding information for $\varkappa_i = 1, \pm 2, -3$ so that all subshells through N_V are represented.

The sum over $\varkappa$ and $\varkappa'$ is now carried out for a fixed pair L, L'. The full notation in which the $\varkappa$ dependence of M_L etc. appears explicitly must now be restored. We define the functions[14]

$$\mathcal{P}_\nu^{\pm}(\vartheta\beta;LL') = P_\nu \pm \sqrt{\frac{(\nu-2)!}{(\nu+2)!}}\,\frac{C(LL'\nu;11)}{C(LL'\nu;1-1)}\,P_\nu^2 \cos 2\beta \qquad (40)$$

In the self terms where $\nu + L + L'$ is even one has

$$\frac{C(LL'\nu;11)}{C(LL'\nu;1-1)} = \sqrt{\frac{(\nu-2)!}{(\nu+2)!}}\;\frac{\left[L(L+1)+L'(L'+1)\right]\nu(\nu+1) - \left[L(L+1)-L'(L'+1)\right]^2}{\nu(\nu+1) - L(L+1) - L'(L'+1)} \qquad (40a)$$

and in the interference terms where $\nu + L + L'$ is odd, the C-coefficient ratio is

$$\frac{C(LL'\nu;11)}{C(LL'\nu;1-1)} = \sqrt{\frac{(\nu-2)!}{(\nu+2)!}}\;(L' - L)(L' + L + 1) \qquad (40b)$$

The cross section now becomes

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[14] Compare L. C. Biedenharn and M. E. Rose, Rev. Mod. Phys. 25, 729 (1953) - especially Eq. (73c).

TABLE I. Final State Angular Momentum Parameters

$s_{\frac{1}{2}}$: $\varkappa_i = -1$, $\ell_{\varkappa_i} = 0$, $\ell_{-\varkappa_i} = 1$, $j_i = \frac{1}{2}$

	$\lambda = L$		$\lambda = L \pm 1$	
$\varkappa$	L+1	-L	-L-1	L
j	L+1/2	L-1/2	L+1/2	L-1/2
$\ell_\varkappa$	L+1	L-1	L	L
$\ell_{-\varkappa}$	L	L	L+1	L-1

$p_{\frac{1}{2}}$: $\varkappa_i = 1$, $\ell_{\varkappa_i} = 1$, $\ell_{-\varkappa_i} = 0$, $j_i = 1/2$

	$\lambda = L$		$\lambda = L \pm 1$	
$\varkappa$	L	-L-1	-L	L+1
j	L-1/2	L+1/2	L-1/2	L+1/2
$\ell_\varkappa$	L	L	L-1	L+1
$\ell_{-\varkappa}$	L-1	L+1	L	L

$p_{3/2}$: $\varkappa_i = -2$, $\ell_{\varkappa_i} = 1$, $\ell_{-\varkappa_i} = 2$, $j_i = 3/2$

	$\lambda = L$				$\lambda = L \pm 1$			
$\varkappa$	L+2	-L-1	L	-L+1	-L-2	L+1	-L	L-1
j	L+3/2	L+1/2	L-1/2	L-3/2	L+3/2	L+1/2	L-1/2	L-3/2
$\ell_\varkappa$	L+2	L	L	L-2	L+1	L+1	L-1	L-1
$\ell_{-\varkappa}$	L+1	L+1	L-1	L-1	L+2	L	L	L-2

TABLE I. (continued)

$d_{3/2}$: $\varkappa_i = 2$, $\ell_{\varkappa_i} = 2$, $\ell_{-\varkappa_i} = 1$, $j_i = 3/2$

	$\lambda = L$				$\lambda = L \pm 1$			
$\varkappa$	-L-2	L+1	-L	L-1	L+2	-L-1	L	-L+1
j	L+3/2	L+1/2	L-1/2	L-3/2	L+3/2	L+1/2	L-1/2	L-3/2
$\ell_\varkappa$	L+1	L+1	L-1	L-1	L+2	L	L	L-2
$\ell_{-\varkappa}$	L+2	L	L	L-2	L+1	L+1	L-1	L-1

$d_{5/2}$: $\varkappa_i = -3$, $\ell_{\varkappa_i} = 2$, $\ell_{-\varkappa_i} = 3$, $j_i = 5/2$

	$\lambda = L$						$\lambda = L \pm 1$					
$\varkappa$	L+3	-L-2	L+1	-L	L-1	-L+2	-L-3	L+2	-L-1	L	-L+1	L-2
j	L+5/2	L+3/2	L+1/2	L-1/2	L-3/2	L-5/2	L+5/2	L+3/2	L+1/2	L-1/2	L-3/2	L-5/2
$\ell_\varkappa$	L+3	L+1	L+1	L-1	L-1	L-3	L+2	L+2	L	L	L-2	L-2
$\ell_{-\varkappa}$	L+2	L+2	L	L	L-2	L-2	L+3	L+1	L+1	L-1	L-1	L-3

$$\sigma_i = -\frac{\pi^2 \alpha n_i}{k} \sum_{LL'\nu} C(LL'\nu;1-1)\left\{ \mathcal{B}_\nu^+ \left[A_\nu(LL') - \bar{C}_\nu(LL')\right] + \mathcal{B}_\nu^- \left[B_\nu(LL') + C_\nu(LL')\right]\right. \tag{41}$$

where

$$A_\nu(LL') = \sum_{\varkappa\varkappa'} (2j+1)(2j'+1)\sqrt{(2\ell_\varkappa+1)(2\ell_{\varkappa'}+1)}\; S_\varkappa S_{\varkappa'} C(\ell_\varkappa\ \ell_{\varkappa'}\ \nu;00)$$
$$W(\ell_\varkappa\ j\ \ell_{\varkappa'} j';\tfrac{1}{2}\nu)W(LjL'j';\tfrac{1}{2}\nu)\ M_L(\varkappa)\ M_{L'}(\varkappa')\cos\phi_{\varkappa\varkappa' LL'} \tag{42}$$

with $\varkappa = L+1, -L$ and $\varkappa' = L'+1, -L'$. The remaining quantities are defined as follows:

$B_\nu(LL')$: In (42) replace $M_L(\varkappa)\ M_{L'}(\varkappa')$ by $E_L(\varkappa)\ E_{L'}(\varkappa')$. Also $\varkappa = -L-1, L$ and $\varkappa' = -L'-1, L'$.

$C_\nu(LL')$: In (42) replace $M_L(\varkappa)\ M_{L'}(\varkappa')\cos\phi$ by $M_L(\varkappa)\ E_{L'}(\varkappa')\sin\phi$ and the permissible values of $\varkappa$, $\varkappa'$ are: $\varkappa = L+1, -L$; $\varkappa' = -L'-1, L'$.

$\bar{C}_\nu(LL')$: In (42) replace $M_L(\varkappa)\ M_{L'}(\varkappa')\cos\phi$ by $E_L(\varkappa)\ M_{L'}(\varkappa')\sin\phi$ with $\varkappa = -L-1, L$ and $\varkappa' = L'+1, -L'$.

In evaluating the quantities A_ν, B_ν, C_ν and $\bar{C}_\nu$ use is made of Table I of BBR to obtain the Racah coefficients and of Eq. (5) of BBR to evaluate ratios of vector addition coefficients. For example, one uses

$$C(L+1,\ L'+1,\ \nu;00) = -\ C(LL'\nu;00)\sqrt{\frac{(L+L'+\nu+2)(L+L'-\nu+1)}{(L+L'+\nu+3)(L+L'-\nu+2)}}$$

and

$$C(L-1\ L'\ \nu;00) = -\ C(L+1,L',\nu;00)\sqrt{\frac{(L+L'+\nu+2)(L+L'-\nu+1)(L'+\nu-L)(L-L'+\nu+1)}{(L+L'+\nu+1)(L+L'-\nu)(L'+\nu-L+1)(L-L'+\nu)}}$$

Inserting the results for A_ν, B_ν, C_ν and $\bar{C}_\nu$ in (41) gives

$$\sigma_i = -\frac{\pi^2 \alpha n_i}{k} \sum_{LL'\nu} \frac{C(LL'\nu;1-1)}{\sqrt{(2L+1)(2L'+1)}}$$

$$\times \Big\{ \mathcal{P}_\nu^+\ C(LL'\nu;00) \Big[(L+L'+\nu+2)(L+L'-\nu+1)\ M_L(L+1)\ M_{L'}(L'+1) \cos\Delta_{L+1,L'+1}$$

$$+ (L+L'+\nu+1)(L+L'-\nu)\ M_L(-L)\ M_{L'}(-L') \cos\Delta_{-L,-L'}$$

$$+ (L-L'+\nu+1)(L'-L+\nu)\ M_L(L+1)\ M_{L'}(-L') \cos\Delta_{L+1,-L'}$$

$$+ (L'-L+\nu+1)(L-L'+\nu)\ M_L(-L)\ M_{L'}(L'+1) \cos\Delta_{-L,L'+1} \Big]$$

$$+ \mathcal{P}_\nu^-\ C(LL'\nu;00) \Big[(L+L'+\nu+1)(L+L'-\nu)\ E_L(L)\ E_{L'}(L') \cos\Delta_{L,L'}$$

$$+ (L+L'+\nu+2)(L+L'+1-\nu)\ E_L(-L-1)\ E_{L'}(-L'-1) \cos\Delta_{-L-1,-L'-1}$$

$$- (L-L'+\nu)(L'-L+\nu+1)\ E_L(L)\ E_{L'}(-L'-1) \cos\Delta_{L,-L'-1}$$

$$- (L'-L+\nu)(L-L'+\nu+1)\ E_L(-L-1)\ E_{L'}(L') \cos\Delta_{-L-1,L'} \Big]$$

$$+ 2\,\mathcal{P}_\nu^-\ C(L+1,L',\nu;00) \sqrt{(L+L'+\nu+2)(L+L'-\nu+1)(\nu+L'-L)(\nu+1+L-L')}$$

$$\times \Big[M_L(-L)\ E_{L'}(-L'-1) \cos\Delta_{-L,-L'-1} - M_L(L+1)\ E_{L'}(L') \cos\Delta_{L+1,L'}$$

$$+ M_L(-L)\ E_{L'}(L') \cos\Delta_{-L,L'} - M_L(L+1)\ E_{L'}(-L'-1) \cos\Delta_{L+1,-L'-1} \Big] \Big\} \qquad (43)$$

Here we have made use of the fact that

$$\bar{C}_\nu(LL') = -\ C_\nu(L'L)$$

and for $L + L' + \nu$ odd

$$\mathcal{P}_{\nu}^{\pm}(LL') = \mathcal{P}_{\nu}^{\mp}(L'L)$$

while, in general,

$$C(LL'\nu;1\text{-}1) = C(L'L\nu;1\text{-}1)$$

It will be noted that, as expressed above, the self terms involving $M_L(\varkappa)\, M_{L'}(\varkappa')$ and $E_L(\varkappa)\, E_{L'}(\varkappa')$ are separately symmetric in L, L'. Therefore the sum over L and L' can be replaced as usual by:

$$\sum_{LL'} = \sum_{L=L'} + 2 \sum_{L>L'}$$

Since there will be a value of L (or L') beyond which the contribution to the cross section is very small,[15] the sums are to be regarded as finite ones and the number of terms involved is $\sim \frac{1}{2} L_{max}^2$. The interference term can be treated in the same way if the C_ν and $\overline{C}_\nu$ terms are not combined. These interference terms then become

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[15] This is clear since the radial matrix elements involve the standing wave cylinder functions, $j_\lambda(kr)$. For increasing L both λ and $|\varkappa|$ increase and the indicial behavior of the integrands of R_λ, $\overline{R}_\lambda$ is $r^{\lambda+\gamma_\varkappa+\gamma_{\varkappa_i}}$. For sufficiently large L, this centrifugal repulsion effect suppresses the contribution from the only region which can contribute effectively: i.e., r not much larger than the radius of the subshell in question.

$$C(L+1,L',\nu;00)\ \sqrt{(L+L'+\nu+2)(L+L'-\nu+1)(\nu+L'-L)(\nu+1+L-L')}$$

$$\times\Big[\mathcal{P}_\nu^-\Big(M_L(-L)\,E_{L'}(-L'-1)\cos\Delta_{-L,-L'-1} - M_L(L)\,E_{L'}(L')\cos\Delta_{L+1,L'}$$

$$+ M_L(-L)\,E_{L'}(L')\cos\Delta_{-L,L'} - M_L(L+1)\,E_{L'}(-L'-1)\cos\Delta_{L+1,-L'-1}\Big)$$

$$+\ \mathcal{P}_\nu^+\Big(E_L(-L-1)\,M_{L'}(-L')\cos\Delta_{-L-1,-L'} - E_L(L)\,M_{L'}(L'+1)\cos\Delta_{L,L'+1}$$

$$+ E_L(L)\,M_{L'}(-L')\cos\Delta_{L,-L'} - E_L(-L-1)\,M_{L'}(L'+1)\cos\Delta_{-L-1,L'+1}\Big)\Big]$$

To make the matrix elements $M_L(\varkappa)$ etc. more explicit the Q-quantities, see Eqs. (32) and (33), may be evaluated. The results are given in Table II. The following relations, which are easily established from the definitions given in II(b), are useful as checks. These relations are valid for all $\varkappa$ values.

For $\lambda = L$

$$Q(\varkappa_1\varkappa_2;LL) = -\,Q(-\varkappa_1-\varkappa_2;LL)$$

$$(L+1-\varkappa_1-\varkappa_2)\,Q(\varkappa_1\varkappa_2;L+1\ L) = (L+1+\varkappa_1+\varkappa_2)\,Q(-\varkappa_1-\varkappa_2;L+1\ L)$$

$$-\,(\varkappa_1+\varkappa_2+L)\,Q(\varkappa_1\varkappa_2;L-1\ L) = (\varkappa_1+\varkappa_2-L)\,Q(-\varkappa_1-\varkappa_2;L-1\ L)$$

$$\sqrt{L+1}\,(\varkappa_1+\varkappa_2-L)\,Q(\varkappa_1\varkappa_2;L+1\ L) = \sqrt{L}\,(\varkappa_1+\varkappa_2+L+1)\,Q(\varkappa_1\varkappa_2;L-1\ L)$$

Further progress depends on the evaluation of the radial integrals. This phase of the calculation will involve the use of the high speed digital computer and discussion of the attendant problems is deferred. The phase shift differences $\Delta_{\varkappa\varkappa'}$ also depend on the radial functions and on the

TABLE II. Q's for $s_{\frac{1}{2}}$ electrons. ($\varkappa_i = -1$)

	$Q(-\varkappa, \varkappa_i;\lambda L)$	$Q(\varkappa, -\varkappa_i;\lambda L)$
Magnetic $\lambda = L$:		
$\varkappa = L+1$	$\sqrt{\frac{L}{4\pi(L+1)}}$	$-\sqrt{\frac{L}{4\pi(L+1)}}$
$\varkappa = -L$	$-\sqrt{\frac{L+1}{4\pi L}}$	$\sqrt{\frac{L+1}{4\pi L}}$
Electric $\lambda = L+1$:		
$\varkappa = -L-1$	$\sqrt{\frac{2L+1}{4\pi(L+1)}}$	$\sqrt{\frac{1}{4\pi(L+1)(2L+1)}}$
$\varkappa = L$	0	$2\sqrt{\frac{L+1}{4\pi(2L+1)}}$
Electric $\lambda = L-1$:		
$\varkappa = -L-1$	0	$2\sqrt{\frac{L}{4\pi(2L+1)}}$
$\varkappa = L$	$-\sqrt{\frac{2L+1}{4\pi L}}$	$\sqrt{\frac{1}{4\pi L(2L+1)}}$

potential V.

The total cross section for an $s_{\frac{1}{2}}$ electron is

$$\bar{\sigma}_i = \frac{8\pi^3 \alpha n_i}{k} \sum_L \frac{1}{2L+1} \Big[(L+1) M_L^2(L+1) + L M_L^2(-L) + (L+1) E_L^2(-L-1) + L E_L^2(L) \Big] \tag{44}$$

It will be seen that not only in the case of an $s_{\frac{1}{2}}$ electron but also in general the matrix elements and radial integrals involved in the polarization-independent and polarization-sensitive parts of the cross-section are the same. Therefore, it is no more difficult to include the polarization than it is to omit it. Nevertheless the computational problem for angular distribution (with or without polarization) is rather formidable unless the radiation energy is low. For all but low energies the effective maximum L will be a fairly large number (say, for one percent accuracy in σ_i) and a double series (LL' summation) is involved. The sum over ν is from 0 (or 2) to 2 L_{max} in the self terms and from 1 to 2 L_{max} - 1 in the interference terms. From the expectation of a strong forward peak for the emitted electrons it appears that fairly large values of ν will be effective. Thus there is a three-fold series to consider. The requirement that ν, L and L' form a triangle will restrict the number of terms. Thus if we assume L, L' $\lesssim L_m$ the number of terms in the triple sum is of order $\frac{1}{3} L_m^3$. However it is important to note that the ν dependence of

the summand is comparatively simple in that no radial integrals are involved.

For the total cross section $\bar{\sigma}_i$ the situation is much simpler. Only a single sum is involved. If in this sum $L \lesssim L_m$ the number of radial integrals involved is $2(2L_m+3) \sim 4L_m$.

APPENDIX

Reduction of the Degenerate X-coefficient

The X-coefficient which appears in (30) arises quite frequently wherever the spin coupling of two $\frac{1}{2}$-spin particles are involved. The appearance of this coefficient in the reduced matrix elements of the Gamow-Teller interaction in β-decay may be noted.[16] Explicit results for this X-coefficient were given in this reference 16 for $\lambda = L$ and $\lambda = L - 1$ and these results could easily be extended to the case $\lambda = L + 1$. However, it is of greater interest to note that this X-coefficient is directly proportional to the simplest non-trivial Racah coefficient. From the result to be obtained here (Eqs. (31)) the values of the X-coefficient are most readily obtained.

The method of reduction of $X(L\bar{j}\bar{j};\lambda\, \ell\, \bar{\ell}\;;1\tfrac{1}{2}\tfrac{1}{2})$ is to recall that this coefficient appeared as the factor of the (reduced) matrix element of the tensor $\vec{\sigma}\cdot\vec{T}^{M}_{L\lambda}$; viz

$$\left\langle \chi^{\mu}_{\varkappa} \,\middle|\, \vec{\sigma}\cdot\vec{T}^{M}_{L\lambda} \,\middle|\, \chi^{\bar{\mu}}_{\bar{\varkappa}} \right\rangle = (-)^{j+\bar{j}+\ell+\bar{\ell}} \sqrt{\frac{3}{2\pi}\,(2\lambda+1)(2L+1)(2\bar{\ell}+1)(2\bar{j}+1)}$$

$$\times\; C(\lambda\bar{\ell}\ell\,;00)\; X(L\bar{j}\bar{j};\lambda\ell\bar{\ell}\;;1\tfrac{1}{2}\tfrac{1}{2})\; C(L\bar{j}j;M\bar{\mu}\mu\,). \qquad \text{(A.1)}$$

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[16] M. E. Rose, Phys. Rev. 93, 1326 (1954). Note that the notation of this reference interchanges λ and L as compared to that used here.

Now it is of interest to note that the set of three tensors $\vec{T}_{L\lambda}$ (λ = L, L $\pm$ 1) can be expressed in another form:

$$\vec{T}^M_{LL} = - \frac{\vec{L}}{\sqrt{L(L+1)}} \quad Y^M_L \tag{A.2}$$

$$\vec{T}^M_{L\ L+1} = \frac{r \nabla Y^M_L - (L+1) \hat{r} Y^M_L}{\sqrt{(L+1)(2L+1)}} \tag{A.3}$$

$$\vec{T}^M_{L\ L-1} = \frac{r \nabla Y^M_L + L \hat{r} Y^M_L}{\sqrt{L(2L+1)}} \tag{A.4}$$

and $\vec{L} = - i \vec{r} \times \nabla$ is the orbital angular momentum operator and $\hat{r}$ is the unit radial vector. The relation between the two representations of the irreducible tensors is discussed at length in R, Chaps. II and III. The proof of (A.2) .. (A.4) is fairly straightforward. We illustrate by considering

$$\hat{r} Y^M_L = \sum_m (-)^m \frac{r_m}{r} \vec{u}_{-m} Y^M_L$$

$$= \sqrt{\frac{4\pi}{3}} \sum_m (-)^m Y^m_1 Y^M_L \vec{u}_{-m}$$

$$= \sum_m (-)^m \left[\sqrt{\frac{L+1}{2L+3}} C(L1L+1;Mm) Y^{M+m}_{L+1} \vec{u}_{-m} \right.$$

$$\left. - \sqrt{\frac{L}{2L-1}} C(L1L-1;Mm) Y^{M+m}_{L-1} \vec{u}_{-m} \right]$$

wherein R – (2.33) and

$$C(L1L+1;00) = \sqrt{\frac{L+1}{2L+1}}$$

$$C(L1L-1;00) = -\sqrt{\frac{L}{2L+1}} \tag{A.5}$$

have been used. Using the symmetry relations of the C-coefficients (RBA, Appendix B) one obtains directly

$$\hat{r}\, Y_L^M = -\sqrt{\frac{L+1}{2L+1}}\ \vec{T}^M_{L,L+1} + \sqrt{\frac{L}{2L+1}}\ \vec{T}^M_{L,L-1} \tag{A.6}$$

From R, Eq. (2.58) we obtain

$$r\,\nabla\, Y_L^M = L\sqrt{\frac{L+1}{2L+1}}\ \vec{T}^M_{L,L+1} + (L+1)\sqrt{\frac{L}{2L+1}}\ \vec{T}^M_{L,L-1} \tag{A.7}$$

and (A.3) and (A.4) follow immediately. (A.2) is easily obtained using the well-known result

$$L_m\, Y_L^M = (-)^m \sqrt{L(L+1)}\ C(L1L;m+M,-m)\ Y_L^{M+m} \tag{A.8}$$

We now calculate the matrix elements of $\vec{\sigma}\cdot\vec{L}\, Y_L^M$, $r\,\vec{\sigma}\cdot\nabla\, Y_L^M$ and $\sigma_r\, Y_L^M$. Thus

$$\langle \chi_\varkappa^\mu | \vec{\sigma}\cdot\vec{L}\, Y_L^M | \chi_{\bar{\varkappa}}^{\bar{\mu}} \rangle = \langle \vec{\sigma}\cdot\vec{L}\, \chi_\varkappa^\mu | Y_L^M | \chi_{\bar{\varkappa}}^{\bar{\mu}} \rangle - \langle \chi_\varkappa^\mu | Y_L^M | \vec{\sigma}\cdot L\, \chi_{\bar{\varkappa}}^{\bar{\mu}} \rangle$$

$$= (\bar{\varkappa} - \varkappa) \langle \chi_\varkappa^\mu | Y_L^M | \chi_{\bar{\varkappa}}^{\bar{\mu}} \rangle \tag{A.9}$$

where $\vec{\sigma}\cdot\vec{L}\,\chi^{\mu}_{\varkappa} = -(\varkappa+1)\chi^{\mu}_{\varkappa}$ has been used. With the identity

$$r\,\vec{\sigma}\cdot\nabla = \sigma_r\left(r\frac{\partial}{\partial r} - \vec{\sigma}\cdot\vec{L}\right) \tag{A.10}$$

and $\sigma_r\chi^{\mu}_{\varkappa} = -\chi^{\mu}_{-\varkappa}$ one finds

$$\left\langle \chi^{\mu}_{\varkappa}\middle| r\,\vec{\sigma}\cdot\nabla Y^M_L \middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle = -\left\langle \chi^{\mu}_{\varkappa}\middle|\sigma_r\,\vec{\sigma}\cdot\vec{L}\,Y^M_L\middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle$$

$$= \left\langle \chi^{\mu}_{-\varkappa}\middle|\vec{\sigma}\cdot\vec{L}\,Y^M_L\middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle = (\bar{\varkappa}+\varkappa)\left\langle \chi^{\mu}_{-\varkappa}\middle| Y^M_L \middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle \tag{A.11}$$

$$\left\langle \chi^{\mu}_{\varkappa}\middle|\sigma_r\,Y^M_L\middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle = -\left\langle \chi^{\mu}_{-\varkappa}\middle| Y^M_L \middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle \tag{A.12}$$

Using the standard procedure for coupling of spherical harmonics and a Racah recoupling we find

$$\left\langle \chi^{\mu}_{\varkappa}\middle| Y^M_L \middle|\chi^{\bar{\mu}}_{\bar{\varkappa}}\right\rangle = \sqrt{\frac{(2L+1)(2\bar{\ell}+1)(2\bar{j}+1)}{4\pi}}\; C(L\,\bar{\ell}\,\ell;00)\; C(L\bar{j}j;M\bar{\mu}\mu)$$

$$\times\; W(L\,\bar{\ell}\,j\tfrac{1}{2};\,\ell\,\bar{j}) \tag{A.13}$$

Substituting (A.9), (A.11) and (A.12) into (A.2), (A.3) and (A.4), using (A.13) and comparing with (A.1) yields the results (31a), (31b) and (31c).